DRAFT 4/97

4.16 Test of Multisolute Transport with Chemical Reaction

This test verifies that FEHM has correctly implemented the transport of multiple, chemically interacting species in solution for a mixed kinetic and equilibrium reaction system. Figure 58 compares the breakthrough curves for aqueous species for FEHM and PDREACT, the code used for the comparison. Figure 59 compares the solid concentrations versus time at the outlet of the system for the two codes. There is excellent agreement between the two codes for this reactive-transport problem. The PDREACT ouput is found in files *multi.pdreact_CoEDTA_aq.out*, *multi.pdreact_CoEDTA_s.out*, *multi.pdreact_Co_aq.out*, *multi.pdreact_Co_s.out*, *multi.pdreact_EDTA_aq.out*, *multi.pdreact_FeEDTA_aq.out*, *multi.pdreact_FeEDTA_s.out*, and *multi.pdreact_Fe_aq.out*. Table 58 indicates that the percent errors of all species at the outlet were less than 6% for concentrations greater than 10% of their peak values. These results meet the acceptance criteria for this test suite developed in Chapter III. Numerical results for aqueous *EDTA* and *Fe* are not considered because the concentrations are very near zero, and at such low concentrations, a good measure of error is not available.

Table 58. Results of the test of multisolute reactive transport

V&V test	Maximum error	Maximum % error	RMS error
Aqueous-species concentration versus time			
Co	0.4797e-05	1.591	0.9782e-03
CoEDTA	0.1389e-03	3.386	0.2229e-02
FeEDTA	0.4176e-04	2.238	0.1602e-02
Solid-species concentration versus time			
Co	0.2270e-04	1.660	0.9846e-03
CoEDTA	0.7516e-04	5.608	0.3216e-02
FeEDTA	0.2771e-04	3.199	0.2135e-02

DRAFT 4/97

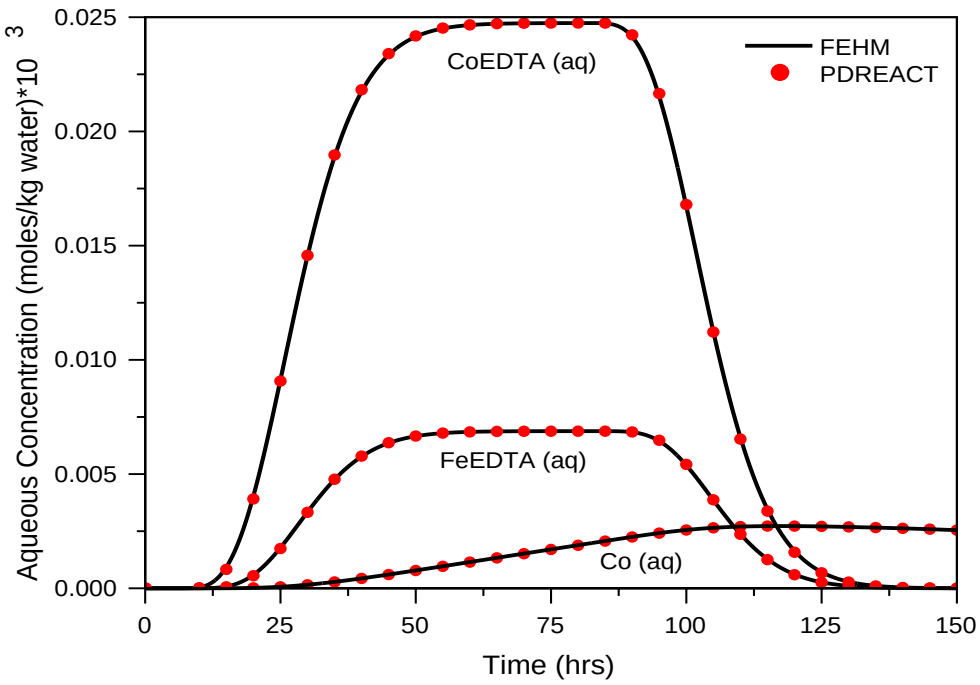

Figure 58. Comparison of FEHM and PDREACT for the breakthrough curves of aqueous species.

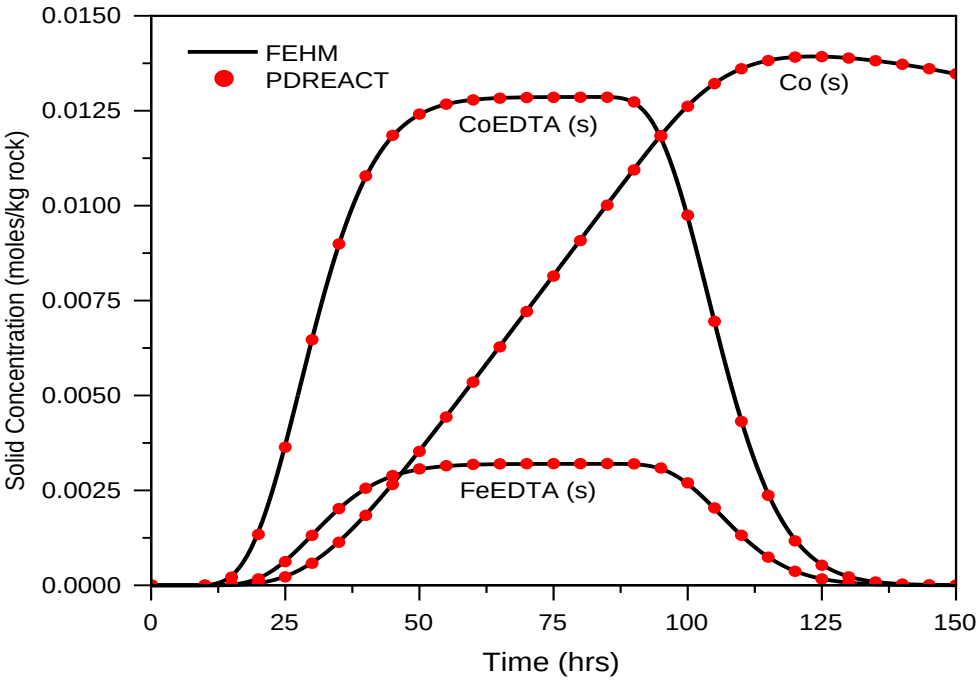

Figure 59. Comparison of FEHM and PDREACT for the exit concentration versus time for solid species.